# Application of a Dispersion Relation to the Electron Impact Widths and Shifts of Isolated Spectral Lines from Neutral Atoms*

H. R. GRIEM
*University of Maryland, College Park, Maryland*
*and*
*U. S. Naval Research Laboratory, Washington, D. C.*

AND

C. S. SHEN†‡
*University of Maryland, College Park, Maryland*

(Received August 9, 1961)

From a quantum mechanical dispersion relation for the scattering amplitudes of thermal electrons on excited states of emitting atoms follows a dispersion relation between electron impact widths and shifts of isolated spectral lines. This relation is used to check the consistency of previous calculations of the impact broadening made with the classical path assumption and to fully determine the parameters for the cutoff at small impact parameters in the usual perturbation theory.

## INTRODUCTION

IN the preceding paper[1] widths and shifts due to electron impacts of isolated, i.e., nonoverlapping lines, were calculated in the classical path approximation for the perturbing electrons, using perturbation theory for distant collisions and an estimate of the Weisskopf type for close collisions. This strong collision term contributes typically 20% to the half-widths, which are therefore not seriously affected by the uncertainties in this term. For the shifts the strong collision contribution is usually neglected, but actually no reliable estimates exist here, and the shifts calculated in the previous paper might therefore have a larger error than the widths.

When also the perturbing electrons are treated quantum mechanically, one finds that electron impact widths and shifts are proportional to the thermal averages of the imaginary and real parts, respectively, of the forward scattering amplitudes for the scattering of single electrons by the excited atoms,[2] if only the perturbation of the upper states is important, and if there is no essential degeneracy, in which case the quantum mechanical result is much more complicated.[2,3] A dispersion relation for scattering amplitudes thus results in a corresponding relation between widths and shifts of isolated lines, as long as the impact approximation is valid. This relation can be used to check the internal consistency of widths and shifts obtained from the classical path approximation, i.e., essentially the consistency of the estimates for the strong collision terms. By requiring that the classical path result fulfills the dispersion relation at least in a certain limit, one can also remove an ambiguity in the determination of the parameters characterizing the strong collision terms.

## DISPERSION RELATION FOR FORWARD SCATTERING AMPLITUDES

For potential scattering, it can be shown that the scattering amplitude obeys the following relation[4,5]:

$$\mathrm{Re}f(\theta,E)=\frac{1}{\pi}P\int_0^\infty \mathrm{Im}f(\theta,E')\frac{dE'}{E-E'} -\sum R_j(E,\theta)-f_B(E,\theta),$$

if the scattering potential is local and central and fulfills

$$\bar{V}(r)\leq m/r^2 \quad \text{for} \quad r\to\infty \quad \text{with} \quad m<\infty,$$

$$\int_0^\infty r\bar{V}(r)dr\leq M<\infty \quad \text{and} \quad \int_0^\infty e^{\alpha r}r^2\bar{V}(r)dr\leq L<\infty.$$

Here $\alpha$ is some positive number which is greater than the momentum transfer

$$\tau=2k\sin(\theta/2)=(2/\hbar)(2mE)^{\frac{1}{2}}\sin(\theta/2).$$

The $R_j(E,\theta)$ are the residues of the function $[f(E',\theta)-f_B(E',\theta)]/(E-E')$ due to poles at $E'=E_j$, with $E_j$ being the energies of bound states of the complete system. Finally, $f_B(E,\theta)$ is the first-order Born approximation for the scattering amplitude.

Potentials of neutral atoms are, in general, not central. But in impact broadening one averages over all directions of the perturbers. The velocity distribution is usually isotropic, and the average over angles thus results in an effective potential that is central.

As mentioned before, in line broadening one is only interested in forward scattering ($\theta=0$). Then the constant $\alpha$ can be put to zero, and practically all potentials

* Supported by the Office of Naval Research.

† This paper is based on a thesis submitted by C. S. Shen in partial fulfillment of the requirements for the degree of Doctor of Philosophy at the University of Maryland, College Park, Maryland.

‡ Now at the Plasma Physics Laboratory, Princeton University, Princeton, New Jersey.

[1] H. R. Griem, M. Baranger, A. C. Kolb, and G. Oertel, preceding paper [Phys. Rev. **125**, 177 (1962)].

[2] M. Baranger, Phys. Rev. **112**, 855 (1958).

[3] M. Baranger, Phys. Rev. **111**, 494 (1958).

[4] N. N. Khuri, Phys. Rev. **108**, 1148 (1957).

[5] A. Klein and C. Zemach, Ann. Phys. **7**, 365 (1959).

would fulfill the above conditions. Furthermore, there is no difficulty associated with cuts in unphysical regions[6] which may be necessary for $\theta \neq 0$, because then the condition $\int_0^\infty e^{\alpha r} r^2 \bar{V}(r) dr \leq L < \infty$, $\alpha \geq \tau$ is not normally satisfied.

The main contribution to the forward scattering of atoms in excited states is from high-$l$ partial waves, for which one can prove using Bargmann's theorem[7] that no bound states exist.[8] This suggests that the residue terms are negligible for the line broadening problem, because for the potentials occurring here one has separate dispersion relations for all partial waves.[9] For lines from neutral atoms this conjecture is substantiated further by the apparent scarcity of excited states of negative ions. (For electron scattering on ground state hydrogen atoms the residue term must be included.[10])

Detailed calculations[8] show that also the first-order Born term can be neglected, which is not too surprising because for electron scattering in the thermal ($\sim$1 ev) range polarization effects are most important. Furthermore, this term obviously depends on the sign of the charge of the perturbers. Therefore, in a plasma, the corresponding ion effects will tend to cancel this term. (It would cause a small shift of the line maximum, where the impact approximation is often valid for both electrons and ions.)

For the present problem, therefore, the following simplified dispersion relation should be applicable:

$$\mathrm{Re} f(0,E) = \frac{1}{\pi} P \int_0^\infty \mathrm{Im} f(0,E') \frac{dE'}{E - E'}.$$

One might suspect that this relation, which was derived for potential scattering, would not hold for situations where polarization or exchange effects are important. However, the structure of the dispersion relation is only determined by the analytic properties of the Green's function of the Hamiltonian describing the scattering[4]; and these analytic properties remain unchanged if the assumption of potential scattering is removed, as long as the interaction falls off rapidly enough that the scattering amplitude is uniformly bounded. (For further discussion on this point see reference 10.)

## DISPERSION RELATION FOR WIDTHS AND SHIFTS

Except for a factor, the shift of an isolated line is given by $\mathrm{Re} f(0,E)$ and the width by $-\mathrm{Im} f(0,E)$ [Eqs. (72a,b) of reference 2], and the appropriate relation between width $w(E)$ and shift $d(E)$ due to impacts with electrons of energy $E$ is therefore

$$|d(E)| = \frac{1}{\pi} \left| P \int_0^\infty \frac{w(E')}{E - E'} dE' \right|.$$

This dispersion relation is obviously fulfilled by the weak collision contributions described by Eq. (3.10) of reference 1, because in this approximation width and shift can be expressed as real and imaginary part of a complex function (Appendix Y of reference 1) having all the required properties.

If now the usual estimate for the contribution of strong collisions (within some impact parameter $\rho_{\min}$) to the width, namely $w_s = \beta N \pi \rho_{\min}^2 v$, with $\beta$ being a parameter of order 1, is adopted, then the dispersion relation requires that half of this term be added to the shift, where the factor $\frac{1}{2}$ arises from the branch cut along the real axis in the $E$ plane. (For mathematical details see Appendix C of reference 8.) Therefore it is consistent with the dispersion relation to assume, leaving out the Maxwell average and using $z_{\alpha\alpha'}{}^{\min} = w_{\alpha\alpha'} \rho_{\min}/v$, that

$$d^D = \tfrac{1}{2} w_s + d_w = \tfrac{1}{2} \beta N \pi \rho_{\min}^2 v + \frac{4}{3} \frac{\pi}{v} \left( \frac{\hbar}{m} \right)^2 N \sum_{\alpha', \sigma} |\langle \alpha | r_\sigma / a_0 | \alpha' \rangle|^2 b(z_{\alpha\alpha'}{}^{\min}),$$

if the width is chosen as

$$w = w_s + w_w = \beta N \pi \rho_{\min}^2 v + \frac{4\pi}{3v} \left( \frac{\hbar}{m} \right)^2 N \sum_{\alpha', \sigma} |\langle \alpha | r_\sigma / a_0 | \alpha' \rangle|^2 a(z_{\alpha\alpha'}{}^{\min}).$$

[Compare with Eq. (3.10) of reference 1.]

That the width is actually the better known quantity is suggested by the fact that the different cutoff procedures yield almost identical answers for it (see the following section). Accordingly, it appears appropriate to compare the various expressions for the line shifts with the result obtained from the dispersion relation in each of these cases in order to estimate the uncertainties in the shifts due to the more or less arbitrary choice of the cutoff and the strong collision term.

## VARIOUS EXPRESSIONS FOR WIDTHS AND SHIFTS

In the preceding paper, two cutoff procedures were employed which both yield the exact result in the low-velocity limit, but only the first procedure reduced also to the high-velocity limit. Even in this case, the parameters of order 1 that have to be introduced were not uniquely determined. This ambiguity can be eliminated by requiring that the dispersion relation be fulfilled at least in the low-velocity limit, in addition to requiring that the proper high- and low-velocity limits are obtained.

If, as in the first procedure in the preceding paper, the

---

[6] R. Blankenbecler, M. L. Goldberger, N. N. Khuri, S. B. Treiman, Ann. Phys. **10**, 62 (1960).
[7] V. Bargmann, Proc. Nat. Acad. Sci. U. S. **38**, 960 (1952).
[8] C. S. Shen, Ph.D. thesis, University of Maryland, College Park, Maryland, 1961 (unpublished).
[9] A. Martin, Nuovo cimento **14**, 403 (1959); **15**, 99 (1960).
[10] E. Gerjuoy and N. A. Krall, Phys. Rev. **119**, 705 (1960).

strong collision contribution to the shift is again absorbed in the weak collision term by reducing here $z_{\alpha\alpha'}{}^{\min}$ by a factor $\delta<1$, then the dispersion relation requires for small velocities [large $z_{\alpha\alpha'}{}^{\min}$, i.e., $b(z)\approx\pi/4z$],

$$d^D=\tfrac{1}{2}\beta N\pi\rho_{\min}{}^2v+\frac{4\pi}{3v}\left(\frac{\hbar}{m}\right)^2 N\sum_{\alpha',\sigma}|\langle\alpha|r_\sigma/a_0|\alpha'\rangle|^2\frac{\pi}{4z_{\alpha\alpha'}{}^{\min}}$$

$$=d_s+d_w=\frac{4\pi}{3v}\left(\frac{\hbar}{m}\right)^2 N\sum_{\alpha'\sigma}|\langle\alpha|r_\sigma/a_0|\alpha'\rangle|^2\frac{\pi}{4\delta z_{\alpha\alpha'}{}^{\min}}.$$

In the same limit [$a(z)=0$], the adiabatic theory result [Eq. (3.14) of reference 1] is preserved only if

$$w_s+w_w+i(d_s+d_w)$$

$$=\beta N\pi\rho_{\min}{}^2v+i\frac{4\pi}{3v}\left(\frac{\hbar}{m}\right)^2 N\sum_{\alpha',\sigma}|\langle\alpha|r_\sigma/a_0|\alpha'\rangle|^2\frac{\pi}{4\delta z_{\alpha\alpha'}{}^{\min}}$$

$$=N\left(\frac{\pi}{2}\right)^{5/3}\frac{\Gamma(\tfrac{1}{3})}{3^{\frac{2}{3}}}\left(\frac{\hbar}{m}\right)^{\frac{1}{3}}v^{\frac{1}{3}}$$

$$\times\left(\sum_{\alpha',\sigma}\frac{1}{\omega_{\alpha\alpha'}}|\langle\alpha|r_\sigma/a_0|\alpha'\rangle|^2\right)^{\frac{2}{3}}(1+i\sqrt{3}).$$

The high-velocity limit comes out automatically because then the strong collision term is negligible. In addition, $\rho_{\min}$ must be defined by an equation corresponding to Eq. (3.16) of reference 1, with the right-hand side being replaced by $\gamma$ and with $B(z)=\pi/4z$ and $A(z)=0$. Then the above conditions reduce to $\beta=4\gamma(\delta^{-1}-1)$, $\beta\gamma^{-\frac{2}{3}}=\Gamma(\frac{1}{3})/2$, and $\gamma^{\frac{1}{3}}\delta^{-1}=\Gamma(\frac{1}{3})\sqrt{\frac{3}{4}}$. With $\Gamma(\frac{1}{3})\approx2.679$, one obtains as the physical ($\beta,\gamma,\delta\approx1$, $\delta<1$) solution $\beta=0.92$ (1.00), $\delta=0.71$ (0.75), and $\gamma=0.57$ (0.63). (The values in parentheses were used in the preceding paper for the calculation of $\langle\alpha|\phi_a|\alpha\rangle_1$.)

For the purpose of discussion, one can now consider a line with only one interacting state. Then one has the following expressions, omitting a common factor $v^{-1}(4\pi/3)(\hbar/m)^2N\sum|\langle\alpha|r_\sigma/a_0|\alpha'\rangle|^2$ and putting $z_{\alpha\alpha'\min}=z_1$, or $z_2$, respectively,

$$w_{1,2}\sim\frac{\beta_{1,2}}{2\gamma_{1,2}}[A^2(z_{1,2})+B^2(z_{1,2})]^{\frac{1}{2}}+a(z_{1,2}),$$

$$d_{1,2}\sim b(\delta_{1,2}z_{1,2}),$$

$$d_{1,2}{}^D\sim\frac{\beta_{1,2}}{4\gamma_{1,2}}[A^2(z_{1,2})+B^2(z_{1,2})]^{\frac{1}{2}}+b(z_{1,2}).$$

The index 1 designates the set of parameters determined above and 2 the set used for the calculation of $\langle\alpha|\phi_a|\alpha\rangle_1$ in the preceding paper [Eq. (3.15) of reference 1]. The $d_{1,2}$ are the shifts resulting from the extension of the perturbation theory result, the $d_{1,2}{}^D$ those obtained by inserting the expressions for the widths into the dispersion relation.

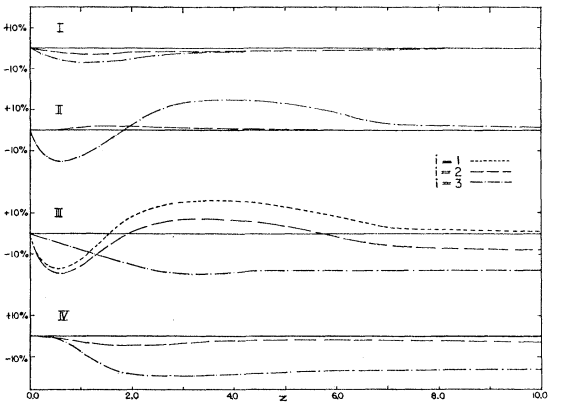


FIG. 1. Comparison of various approximations for electron impact widths ($w_i$ from perturbation theory) and shifts ($d_i$ from perturbation theory, $d_i{}^D$ from $w_i$ using the dispersion relation). I: $(w_1-w_i)/w_1$; II: $(d_1-d_i)/w_1$; III: $(d_i-d_i{}^D)/w_1$; IV: $(d_1{}^D-d_i{}^D)/w_1$.

Furthermore, corresponding to Eq. (3.17) of reference 1, there is another set [$\beta_3=(\frac{4}{3})^{\frac{2}{3}}$, $\gamma_3=\sqrt{\frac{3}{2}}$]:

$$w_3\sim2^{\frac{1}{3}}3^{-7/6}[A^2(z_3)+B^2(z_3)]^{\frac{1}{2}}+a(z_3),$$

$$d_3\sim2^{\frac{1}{3}}3^{-\frac{1}{2}}b(z_3),$$

$$d_3{}^D\sim2^{\frac{1}{3}}3^{-7/6}[A^2(z_3)+B^2(z_3)]^{\frac{1}{2}}+b(z_3).$$

The $z_1$, $z_2$, $z_3$ are not independent of each other, but must be chosen to correspond to the same velocity before intercomparison can be made. According to Eq. (3.16) of reference 1 (modified for general $\gamma$), one must therefore require

$$\gamma_1{}^{-1}z_1{}^{-2}[A^2(z_1)+B^2(z_1)]^{\frac{1}{2}}=\gamma_2{}^{-1}z_2{}^{-2}[A^2(z_2)+B^2(z_2)]^{\frac{1}{2}}$$
$$=\gamma_3{}^{-1}z_3{}^{-2}[A^2(z_3)+B^2(z_3)].$$

From the properties of the functions $A(z)$ and $B(z)$ [see Eq. (Y.17) of reference 1] follows then $z_{2,3}=z_1(\gamma_1/\gamma_{2,3})^{\frac{1}{2}}$ for small $z$ and $z_{2,3}=z_1(\gamma_1/\gamma_{2,3})^{\frac{1}{3}}$ for large $z$, if one wants to use $z_1$ as independent variable.

## RESULTS AND DISCUSSION

Numerical calculations showed that the three expressions for the line width yield the same result over the whole velocity range within about 5% (see Fig. 1). It is therefore convenient to express the deviations of the various shifts from each other in terms of, e.g., the width $w_1$. The resulting percentage deviations are also shown in Fig. 1. They are larger as for the widths, namely range up to ~15%, if one compares the differences of shifts obtained from the extended perturbation theory ($d_1,d_2,d_3$), and up to ~20%, if one wants to check the consistency of these shifts with those calculated from widths using the dispersion relation ($d_1{}^D,d_2{}^D,d_3{}^D$).

None of the expressions considered here appears to be significantly more consistent with the dispersion relation

than the other two.[11] Accordingly, one must expect uncertainties in the shifts of the order of 20% of the (half) half-widths, if one calculates them from the perturbation expansion with a cut-off impact parameter and an estimate for the strong collision term. One might be tempted to overcome this difficulty by using instead one of the shifts obtained from the dispersion relation, because the widths substituted into this relation agreed rather well with each other. However, also these shifts deviate from each other by up to 20% in the region of interest (Fig. 1), again in terms of the width $w_1$.

[11] There are certainly procedures that are consistent with the dispersion relation, e.g., that of Vainshtein and Sobel'man (reference 38 of the preceding paper) who would write the complete damping constant $w+id$ as an analytic function of our $A(z)+iB(z)$. However, the choice of this analytic function is not unique, and the results are therefore not necessarily more accurate than those obtained with the procedures used in reference 1, which are more convenient numerically.

PHYSICAL REVIEW VOLUME 125, NUMBER 1 JANUARY 1, 1962

# Measurement of Stark Profiles of Neutral and Ionized Helium and Hydrogen Lines from Shock-Heated Plasmas in Electromagnetic T Tubes*

H. F. Berg,†‡ A. W. Ali,§ R. Lincke, and H. R. Griem
*University of Maryland, College Park, Maryland*

(Received August 9, 1961)

The slab of plasma behind primary or reflected shock fronts served as thermal light source. Electron densities were determined from absolute continuum intensities. Temperatures in helium followed from intensity ratios of ion and neutral lines, or at lower temperatures and in hydrogen from relative line and continuum intensities. Line profiles were measured by scanning with monochromators from shot to shot. Experimental widths and shifts were compared with values calculated from measured electron densities and temperatures. For hydrogen ($H_\alpha$,$H_\beta$,$H_\gamma$), neutral helium (5876, 5016, 4713, 4471, 3889, 3188A) and ionized helium (4686, 3203A), the widths agree within 10% with theory. He II 4686A exhibits a blue-shift, probably due to the polarization of the plasma near the emitting ions. The measured shifts of the neutral helium lines tend to be smaller than the calculated values, and the agreement with calculated shifts is poorer than in case of the widths.

## INTRODUCTION

In dense plasmas with temperatures in the 1–10 ev range, the dominant line-broadening mechanism is Stark broadening caused by electric microfields from electrons and ions surrounding the emitting atoms or ions. The resulting Stark profiles depend almost exclusively on the electron (ion) density, and are only weak functions of the temperature. Thus, measured Stark profiles can be used to determine electron densities also in situations where the temperature is only approximately known, or even when the existence of a temperature is questionable.

In precision experiments, the accuracy of such electron density measurements is limited by the uncertainties in the theory of Stark broadening, which have been reduced considerably in the past years. For hydrogen,[1–3] neutral helium,[4] and ionized helium[5] lines the errors introduced by the various approximations in the theory are estimated to correspond to 10 or 20% uncertainties in the electron densities. This should be compared with the limiting precision of 5% for electron densities from absolute continuum intensity measurements in the visible, which is mainly determined by the accuracy of presently available intensity standards. (Microwave methods are not applicable to the dense plasmas considered here.)

Both the Stark broadening and the continuum intensity method will have the cited accuracies only if wave functions are exactly known (hydrogen and ionized helium), or at least with a precision that is commensurate with that of the rest of the theory (neutral helium). For this reason, calculations and measurements were first performed for these cases, and the motivation of this experiment was to check to what extent the theoretically estimated accuracies

* Jointly supported by the Geophysics Research Directorate of the Air Force, the Office of Naval Research and the National Science Foundation.

† Now at the National Bureau of Standards.

‡ Some of the material in this article is part of a thesis submitted by H. F. Berg in partial fulfillment of the requirements for the Degree of Doctor of Philosophy at the University of Maryland, College Park, Maryland.

§ This paper also contains some of the material in a thesis submitted by A. W. Ali in partial fulfillment of the requirements for the Degree of Master of Science at the University of Maryland, College Park, Maryland.

[1] H. R. Griem, A. C. Kolb, and K. Y. Shen, Phys. Rev. **116**, 4 (1959).

[2] B. Mozer, Ph.D. thesis, Carnegie Institute of Technology, Pittsburgh, Pennsylvania, 1960 (unpublished).

[3] H. R. Griem, A. C. Kolb, and K. Y. Shen, Astrophys. J. (January 1962).

[4] H. R. Griem, M. Baranger, A. C. Kolb, and G. Oertel, this issue [Phys. Rev. **125**, 177 (1962)].

[5] H. R. Griem, and K. Y. Shen, Phys. Rev. **122**, 1490 (1961).